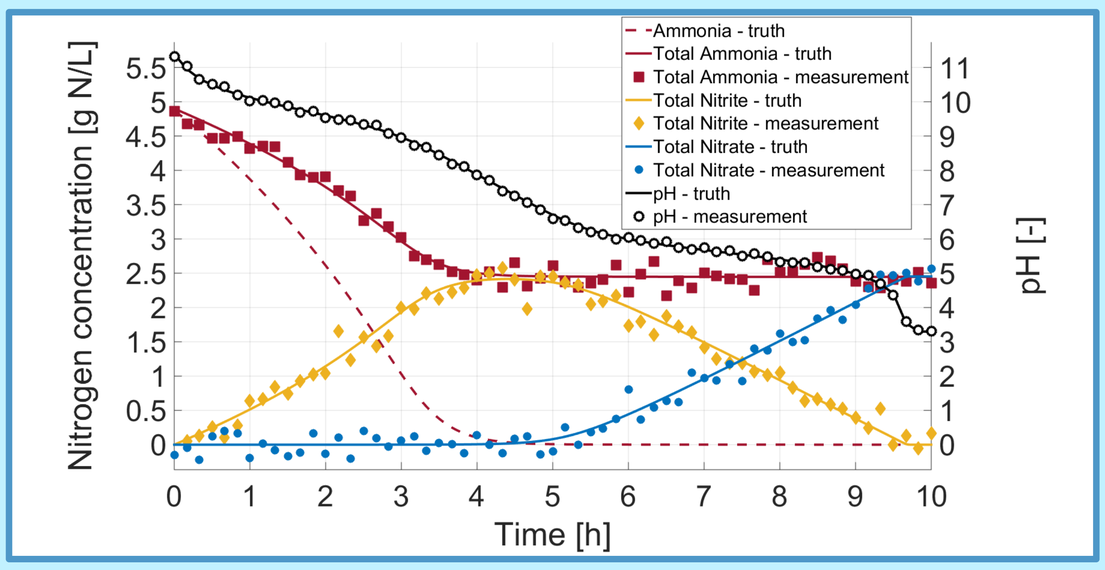
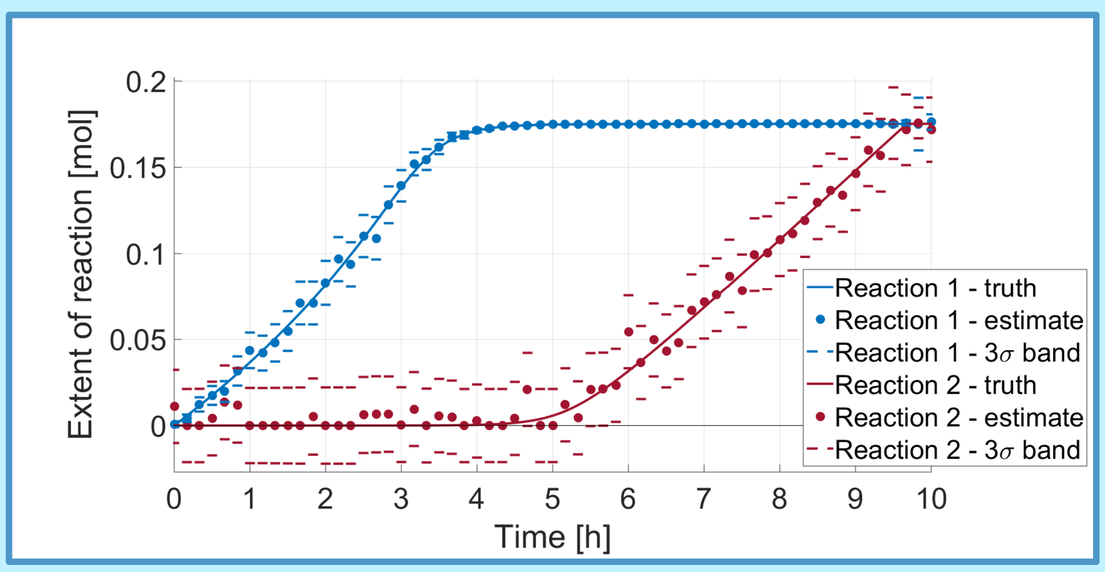
Eawag –
Swiss Federal Institute of Aquatic
Science and Technology

Biokinetic model identification via extents of reaction

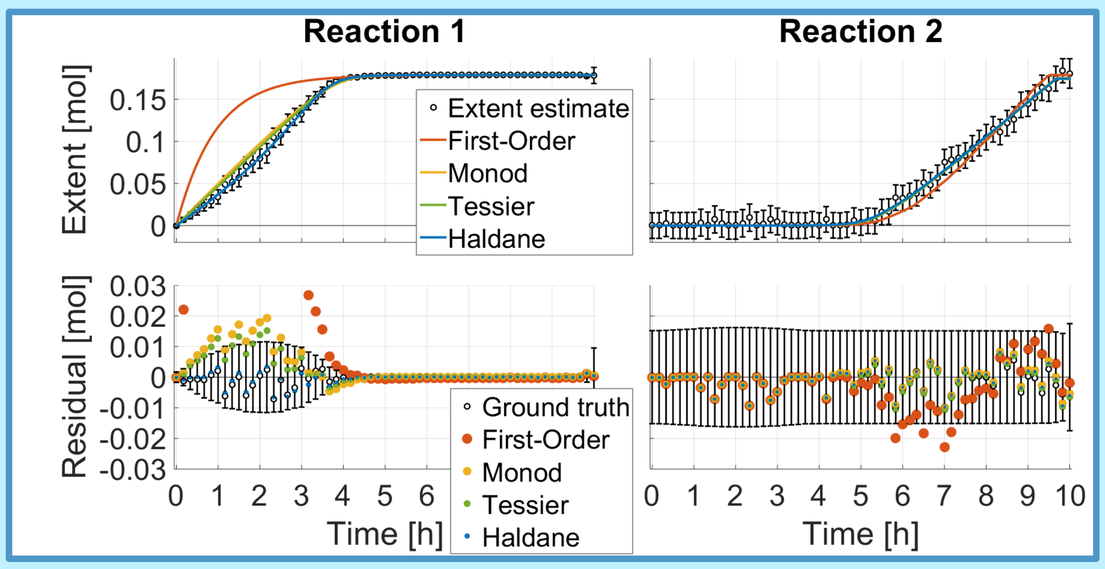
METHOD DEVELOPMENT – SIMULATION



SIMULATION. Measurements of pH and concentrations of total ammonia, total nitrite, and nitrate in a two-step batch nitrification process.

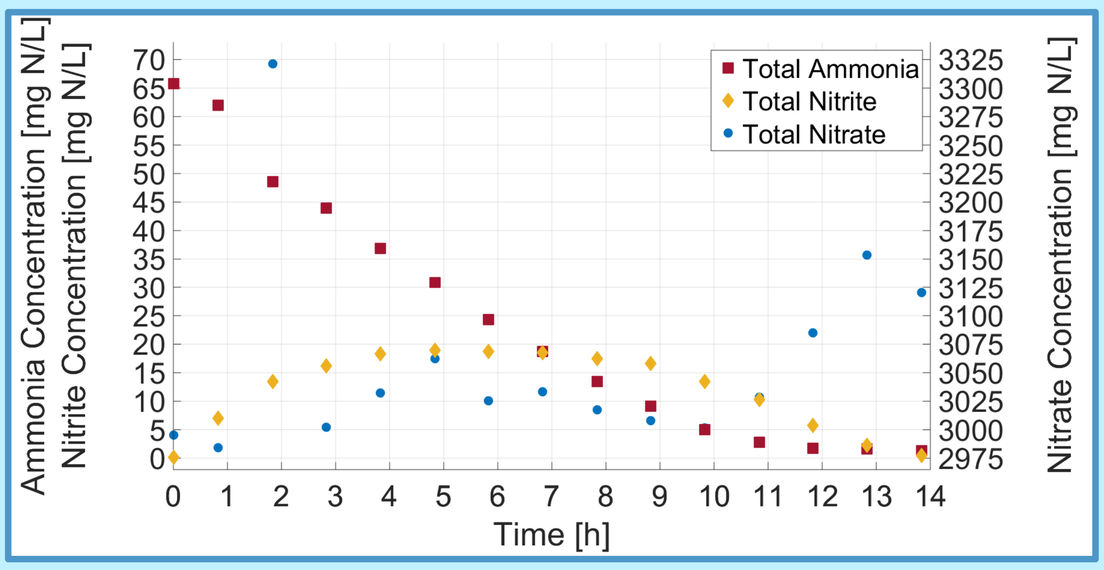


AN EXTENT OF REACTION expresses, in moles, the progress of a single reaction. They are obtained from measurements by means of conservation balances and equilibrium equations.

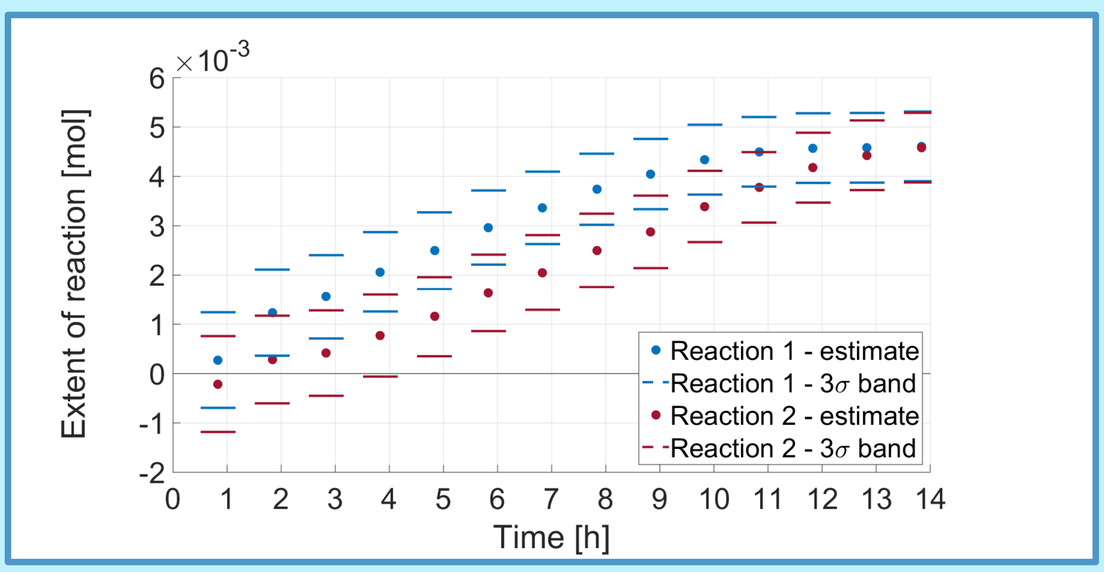


EACH EXTENT CAN BE MODELLED SEPARATELY. The parameters of 4 candidate rate laws are estimated separately for each reaction. This means only 4x2=8 parameter sets are optimized instead of 4^2=16 parameter sets. Which rate laws would you choose?

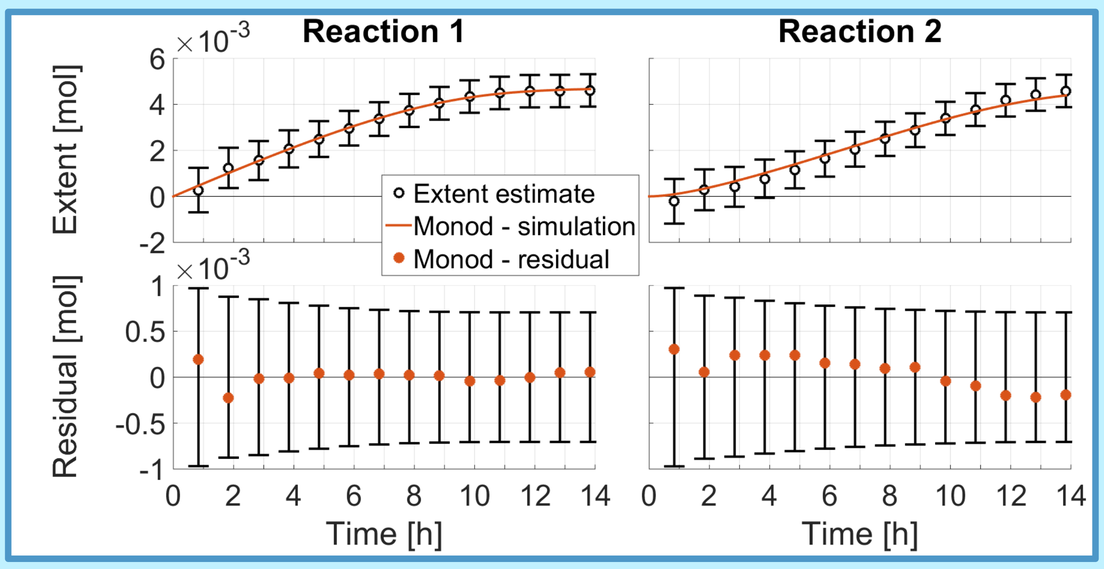
EVALUATION – FIRST EXPERIMENT



MEASUREMENT CAMPAIGN. Measurements of ammonia, nitrite, and nitrate during a cycle of a urine nitrification process for fertilizer production.



EXTENTS OF REACTION. The precision of the estimates is rather low. Improvement is expected following inclusion of further measurements, e.g., pH (as on the left), dissolved oxygen, and UV-Vis spectra.



CURRENT MODEL. The 2 parameters of a Monod rate law are estimated for each reaction separately, instead of estimating the 2x2=4 parameters simultaneously. Are the fitted rate laws acceptable? Should alternative rate laws be tried out?

TAKE HOME

Computation of extents ⟹

- **Facilitates model diagnostics**
- **Speeds up model identification**

TAKE HOME

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